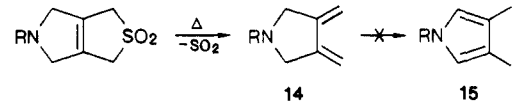
cyclohexane ring and oxoalkyl-substituted cyclopentene, cyclohexene, and pyrrole derivatives.

Clarification of the reaction mechanism is an interesting subject of a further study. One possible reaction path[2,10] is depicted in Scheme I. The strained 1,2-bis(alkylidene)cycloalkane intermediates **3** and **12** are transformed into various cyclic products **6–9** via different hydrogen transfer isomerizations.

The 400 MHz ^{1}H NMR spectra of the bicyclic α-pyrans **6b–e** show that they are sterically congested molecules, in which the free rotation of the ethyl group on the 2-C atom is restricted. Thus the methylene hydrogen atoms H_B and H_C (Scheme I) of **6b–e** are not equivalent (J_{BC} = 14–15 Hz) and exhibit the different coupling constants (J = 9 and 3 Hz) to the methine hydrogen H_A, which appears as a broad doublet (J = 9 Hz). Furthermore, the methylene hydrogens of the ethyl group on the 5-C atom of **6e** are not equivalent. The free rotation of the butyl group on the 5-C atom of **6f** is also restricted. However, it may be inferred that, in comparison with the dienone **11** which is a highly strained molecule owing to the steric repulsion arising from H vs O, H vs R^2, R^1 vs O, or R^1 vs R^2, the bicyclic α-pyrans **6b–f** are relatively stable and can exist without undergoing the ring-opening isomerization to **11**.

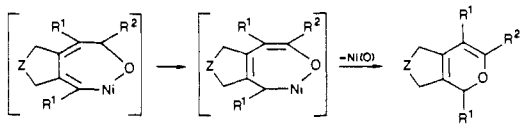
The formation of **7** from the unsubstituted diyne **1a** indicates that an alkyl substituent is necessary at least on the 5-C atom for the existence of the bicyclic α-pyran **6** (Z = CH_2CH_2). The transformation of **6** (Z = CH_2 and ^{n}PrN) to **8** and **9** via the dienone key intermediate **12**[11] (Z = CH_2 and ^{n}PrN) suggests that the α-pyran ring fused with a five-membered ring is unstable and undergoes the electrocyclic ring cleavage to the dienone. The conjugated δ-amino-α,β,γ,δ-dienone intermediate **13** may play an important role in the formation of **9** because it is known that 3,4-dimethylenepyrrolidine (**14**) does not isomerize to 3,4-dimethylpyrrole (**15**)[12] (eq 4).



14 15 (4)

Supplementary Material Available: Typical experimental procedures and characterization (IR, ^{1}H NMR, ^{13}C NMR, MS, and HRMS) data for the products **6a–f** and **7–9** listed in Table I (5 pages). Ordering information is given on any current masthead page.

(10) Another possible reaction path may be the one involving the hydrogen transfer isomerization via a metallacycle containing the nickel atom: for example



10 6

(11) Equilibration of **12** (Z = CH_2 and ^{n}PrN) ⇌ **6** (Z = CH_2 and ^{n}PrN) may be possible.[8b]

(12) Ottenbrite, R. M.; Alston, P. V. *J. Org. Chem.* **1974**, *39*, 1115.

Additions and Corrections

pH Dependence of the Mechanism of Hydrolysis of Benzo[*a*]pyrene-*cis*-7,8-diol 9,10-Epoxide Catalyzed by DNA, Poly(G), and Poly(A) [*J. Am. Chem. Soc.* **1987**, *109*, 2108–2111]. NAFISA B. ISLAM, DALE L. WHALEN,* H. YAGI, and DONALD M. JERINA

Page 2109, Table I: The values of k_{cat}^H (M^{-1} s^{-1}) and k_{cat}^0 (s^{-1}) for the reaction of **DE-1** in solutions of Poly(G) should be >6.3 × 10^5 and >0.20, respectively, and not <6.3 × 10^5 and <0.20 as reported.

Reaction of Dinitrogen Pentoxide with Fluoranthene [*J. Am. Chem. Soc.* **1986**, *108*, 4126–4132]. BARBARA ZIELINSKA,* JANET AREY, ROGER ATKINSON, THOMAS RAMDAHL, ARTHUR M. WINER, and JAMES N. PITTS, JR.

The ^{1}H NMR spectrum reported for 1,2,5-trinitrofluoranthene was actually that of 2,3,5-trinitrofluoranthene. The correct ^{1}H NMR spectrum of 1,2,5-trinitrofluoranthene is as follows ($CDCl_3$): δ 8.95 (d, 1, $J_{(4,6)}$ = 1.6 Hz, C_6H), 8.85 (s, 1, C_3H), 8.83 (d, 1, C_4H), 8.02 (d, 1, $J_{(7,8)}$ = 6.4 Hz, C_7H), 7.86 (d, 1, $J_{(9,10)}$ = 7.6 Hz, $C_{10}H$), 7.63 (t, 1, C_8H), 7.55 (t, 1, C_9H). Both trinitrofluoranthenes are formed in the reaction of 2-nitrofluoranthene with N_2O_5 in CCl_4 solution, with 1,2,5-trinitrofluoranthene being the major trinitro isomer formed.

Computer Software Reviews

Number Cruncher Statistical System. Version 5.01. Dr. Jerry L. Hintze: 865 East 400 North, Kaysville, UT 84037. List price $99.00. Optional NCSS 5.1 Graphics ($59.00) and NCSS 5.3 Power Pack ($49.00) require NCSS 5.0.

Number Cruncher Statistical system (NCSS) is an advanced statistical analysis software package. The program requires an IBM-PC, XT, AT, or close compatible machine. NCSS 5.1 Graphics is an integrated statistical analysis and graphics accessory for NCSS and requires a CGA, EGA, VGA, and Hercules compatible graphics board and was designed to output to an HP-compatible plotter. Other plotters require special drivers, not supplied by NCSS. NCSS Power Pack is an accessory designed to perform advanced statistical procedures. This review was conducted on a Leading Edge Model D (8088, 4.7 MHz) and an Acer 1100 (80386, 16 MHz) equipped with an HP Color Pro Plotter.

The basic NCSS package comes on three 360 Kb floppy disks and is designed to run on either a floppy-disk or hard-disk system with at least 450 Kb of memory. NCSS Graphics needs 512 Kb of memory, two floppy disk drives or a hard-disk, and graphics equipment. NCSS is not copy protected.

NCSS offers a surprising repertoire of statistical techniques, probably well in excess of the needs of the average chemist. At first glance, the organization of the package seems lacking. However, the sheer volume of features presented in NCSS is probably to blame, and closer examination reveals a simply organized system centered around a transfer menu packed with options. A statement of the organizational scheme of the program early in the manual would alleviate this confusion, although this is not a serious flaw. The documentation is otherwise straightforward and able to be followed even by the computer novice. The statistical options of NCSS are thoroughly described, with tutorials for the major features appended. Installation is accomplished easily and quickly by